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Low Energy Positron Interactions with Biological Molecules[1]
INDIKA WANNIARACHCHI, CAROLINE MORGAN, Department of Physics and Astronomy, Wayne State University, Detroit, MI 48202 USA, BERNHARD SCHLEGEL, Department of Chemistry, Wayne State University, Detroit, MI 48202 USA, GARY KEDZIORA, DoD Supercomputing Resource Center (DSRC), Air Force Research Laboratory, 2435 Fifth Street, Bldg 676, Wright-Patterson Air Force Base, OH 45433 USA, LARRY BURGRRAF, Air Force Institute of Technology, AFIT/ENP, 2950 Hobson Way, Wright-Patterson Air Force Base, OH 45433 USA, MICHAEL PAK, SHARON HAMMES-SCHIFFER, Chemistry Department, Penn State Univ., University Park, PA 16802 — There is some experimental evidence that positrons can produce distinctive molecular fragmentation patterns. It is known that tuning the incident positron energy to near resonance with molecule vibrations can strongly enhance the positron annihilation probability for a molecule. This suggests that fragmentation induced by slow positrons may provide valuable complementary information to existing techniques for identification and study of proteins. In order to study this concept, we are developing a general quantum method for reliably calculating the density distribution for positrons bound to large biological molecules using NEO/GAMESS. We find that the outer molecular orbitals as well as the higher p orbitals on the O atoms contribute heavily to the total annihilation rate. Using the basis sets and approximations we have tested to predict where annihilation occurs can ultimately help us understand the resulting fragmentation patterns of larger biological molecules.

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